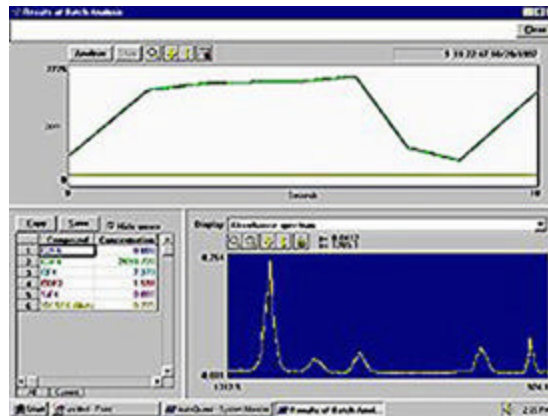


FACT SHEET

Software Improvements to a Fourier Transform Infrared (FTIR) Spectrometer



Improved vapor monitoring software is the result of a nonreimbursable Space Act Agreement between NASA at Kennedy Space Center (KSC) and the MIDAC Corporation of Irvine, California.

The agreement resulted in a commercial software package that gives everyone the ability to make more accurate measurements of chemical compounds using Fourier Transform Infrared Spectrometers (FTIRs). An FTIR detects gases by detecting the frequencies at which gas absorbs light. The usual output is a spectrum that shows frequency (or wave number). By analyzing the peaks and valleys in the data, one can determine what compounds are present. If the baseline of the spectrum is tilted or shifted upward by contamination or during instrument warm-up, accuracy is degraded.

The new software addressed these baseline problems and provided correction to the data. The agreement called for the development of a commercial package and graphical user interface for the software provided by NASA. In return, NASA received copies of the commercial software for use at KSC.

KSC engineers use an FTIR for contamination and toxic vapor detection. Sample measurements are produced in raw form by the FTIR. The basic data is fed into a computer to transform the raw interferogram into sample concentration. The Space Act Agreement called for the development of a system to monitor ammonia vapor in the Space Station Processing Facility (SSPF). Ammonia, though both toxic and flammable, is used as a refrigerant in the International Space Station.

Contamination Monitoring Laboratory (CML) engineers installed and programmed a small computer inside a MIDAC FTIR, and developed new algorithms for the FTIR to recognize and measure various infrared active gasses. The software was compiled and embedded into the computer in the FTIR, producing a customized package for specific job requirements.

The technology has been applied to three KSC Shuttle and payload monitoring systems. KSC's CML designed, fabricated, and delivered a Portable Ammonia Monitoring System using the new software. This new Ammonia Detection Cart has been used during validation testing of the Ammonia Servicer in the SSPF. This servicer contains and controls the ammonia loaded into Space Station elements. The cart has also demonstrated capabilities for detecting alcohols, Freons, ketones, water vapor, and carbon dioxide. The FTIR was also used in the detection carts developed for dimethylethoxysilane (DMES), a waterproofing agent used on Space Shuttle thermal tiles. The NASA FTIR software was further modified for the hydrocarbon monitoring system developed for and used during processing of the Chandra X-ray Observatory at KSC.

The Space Act Agreement allows the software to be polished into a commercial-grade product, of value to both NASA and MIDAC. The commercial software package has been furnished to NASA and is also incorporated in the MIDAC line of products.

AutoQuant from MIDAC Corporation provides an integrated software platform for the automatic collection, archiving, and real-time analysis of FTIR spectral data. The workhorse at the heart of the AutoQuant is an advanced multivariate "classical least squares" (CLS) algorithm developed by NASA scientists at KSC. Mr. Gerald Auth of MIDAC states the modifications by NASA scientists provide a higher degree of "effective stability" and accuracy than is possible with any other commercially available FTIR. He says AutoQuant's power and elegant simplicity have helped to transform the FTIR from a laboratory research instrument into a simple robust gas monitor. Commercially, the FTIRs were first used in laboratories as analytical instruments. They are now being applied to on-line process monitoring.

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